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Synthesis and Structural Characterization of Mononuclear Iron (II) Ferracarboranes

by
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Neutral iron(II) ferracarboranes of the type [*closo*-3-CO-3-L-3-L′-3,1,2-$FeC_2B_9H_{11}$] (**3**, L = CO, L′ = PPh_3; **4**, L = PPh_3, L′ = CH_3CN; **5**, L = CO, L′ = CH_3CN; **6**, L = CO, L′ = $P(OCH_3)_3$; **7**, L = L′ = $P(OCH_3)_3$; **8**, L = L′ = CO) have been prepared by the Cu(I) oxidation of the dimeric iron dicarbollide complex [*closo*-3-CO-3,3′-(μ-CO)-3,1,2′-$FeC_2B_9H_{11}]_2^{2-}$ (**2**) in the presence of the designated monodentate ligands. Complexes **3**, **4**, **7**, and **8** have been structurally characterized by single-crystal X-ray diffraction. Crystallographic parameters are as follows (compound: crystal system; space group; crystal parameters; Z; unique data ($I > 3\sigma(I)$); R,R_w). **3**: monoclinic; $A2/a$; a = 18.384 (3) Å, b = 12.762 (2) Å, c = 23.059 (3) Å, β = 104.081 (4)°; 8; 1780; 7.4, 8.8. **4**: monoclinic; $C2/c$; a = 28.050 (2) Å, b = 11.5715 (9) Å, c = 19.042 (2) Å, β = 116.846 (2)°; 8; 1702; 6.5, 7.7. **7**: orthorhombic; $Pbnm$ (standard setting $Pnma$); a = 10.397 (2) Å, b = 14.419 (3) Å, c = 15.092 (3) Å; 4; 1051; 7.1, 8.9. **8**: monoclinic; $P2_1/n$; a = 6.971 (4) Å, b = 15.900 (9) Å, c = 11.237 (7) Å, β = 91.42 (2)°; 4; 1108; 6.2, 7.4. The closo 12-vertex icosahedral geometry comprising a polyhedral (d^6Fe)C_2B_9 framework and the pseudooctahedral coordination exhibited by the iron atom are common structural features displayed by all four ferracarboranes.

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